

Pentachloroethane
76-01-7 | DTXSID7021104

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.17 days

Global applicability domain: Inside

Local applicability domain index: 4.65e-01

Confidence level: 7.36e-01

Nearest Neighbors from the Training Set

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1,1-Dimethylcyclopentane

Measured: 880

Predicted: 10.9

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1,2,3,4-Tetramethylbenzene

Measured: 24.3

Predicted: 3.95

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1,2,4,5-Tetramethylbenzene

Measured: 88.3

Predicted: 5.46

Image not found

1,2,3-Trimethylbenzene

Measured: 24.3

Predicted: 4.97

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1,2,3,5-Tetramethylbenzene

Measured: 12.5

Predicted: 3.31